



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:27 AM GMT

PDB ID : 3LWL  
Title : Structure of Klenow fragment of Taq polymerase in complex with an abasic site  
Authors : Marx, A.; Diederichs, K.; Obeid, S.  
Deposited on : 2010-02-24  
Resolution : 2.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

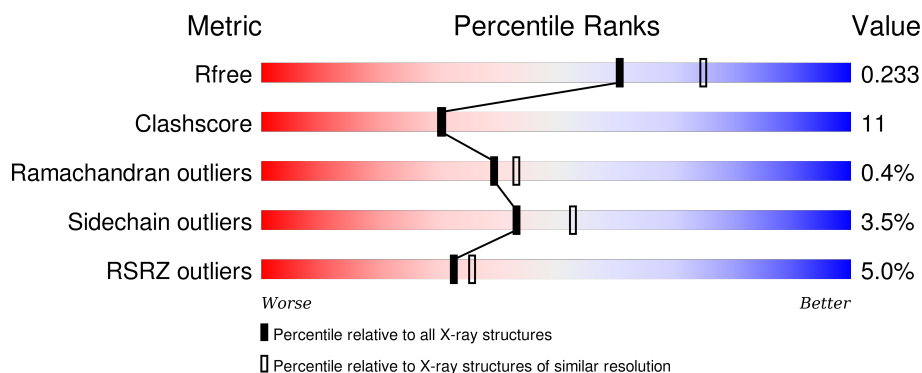
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	540	<div> <div>5%</div> <div>75%</div> <div>22%</div> <div>..</div> </div>
2	B	12	<div> <div>75%</div> <div>17%</div> <div>8%</div> </div>
3	C	16	<div> <div>38%</div> <div>44%</div> <div>6%</div> <div>13%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	ACT	A	5	-	-	-	X
6	ACT	C	6	-	-	-	X
7	GOL	A	6	-	-	X	X
7	GOL	A	835	-	-	-	X
7	GOL	A	836	-	-	-	X
7	GOL	B	8	-	-	X	X
8	NA	A	4	-	-	-	X
8	NA	A	837	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5013 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA polymerase I, thermostable.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	0	0	0
			4236	2693	765	765	13			

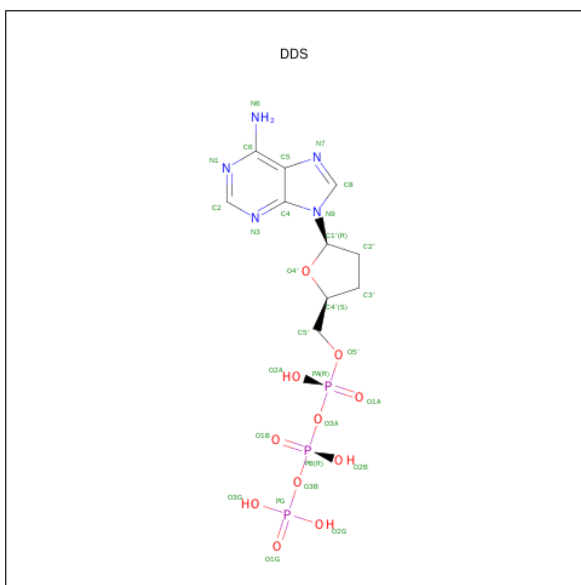
- Molecule 2 is a DNA chain called DNA (5'-D(\*GP\*AP\*CP\*CP\*AP\*CP\*GP\*GP\*CP\*GP\*CP\*(2DA))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	12	Total	C	N	O	P	0	0	0
			242	115	50	66	11			

- Molecule 3 is a DNA chain called DNA (5'-D(\*AP\*AP\*AP\*(3DR)P\*TP\*GP\*CP\*GP\*CP\*CP\*GP\*TP\*GP\*GP\*TP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	14	Total	C	N	O	P	10	0	0
			278	131	48	85	14			

- Molecule 4 is 2',3'-DIDEOXYADENOSINE TRIPHOSPHATE (three-letter code: DDS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>11</sub>P<sub>3</sub>).

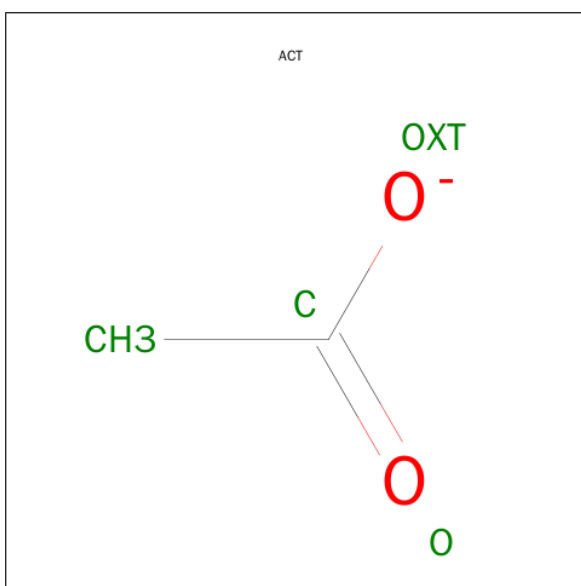


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			29	10	5	11	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

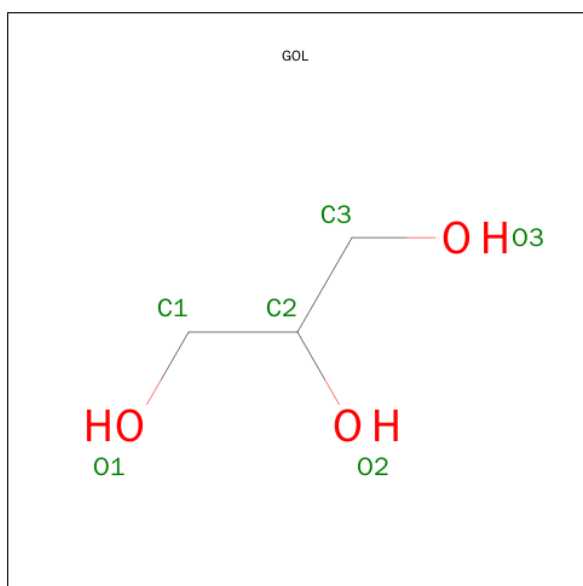
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula:  $\text{C}_2\text{H}_3\text{O}_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	4	Total 4	Na 4	0	0

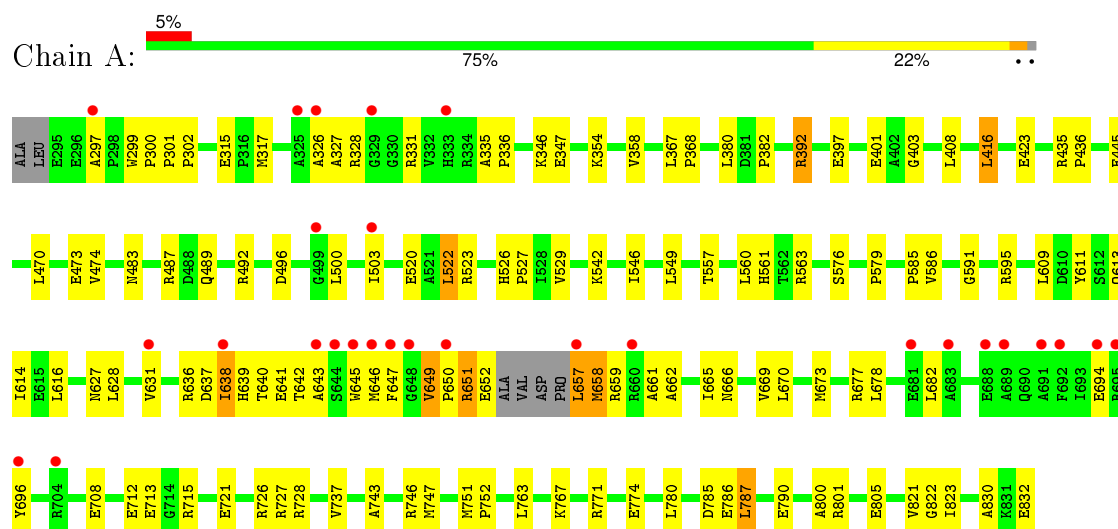
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	112	Total 112	O 112	0	0
9	B	23	Total 23	O 23	0	0
9	C	26	Total 26	O 26	0	0

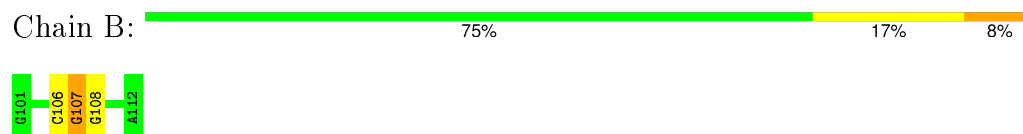
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA polymerase I, thermostable



- Molecule 2: DNA (5'-D(\*GP\*AP\*CP\*CP\*AP\*CP\*GP\*GP\*CP\*GP\*CP\*(2DA))-3')



- Molecule 3: DNA (5'-D(\*AP\*AP\*AP\*(3DR)P\*TP\*GP\*CP\*GP\*CP\*CP\*GP\*TP\*GP\*GP\*TP\*C)-3')





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.23 Å   110.23 Å   91.27 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	47.73 – 2.25 47.73 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.73-2.25) 99.8 (47.73-2.25)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 2.24 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6 _289)	Depositor
R, $R_{free}$	0.188 , 0.234 0.187 , 0.233	Depositor DCC
$R_{free}$ test set	1560 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.1	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.4	EDS
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 30732 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5013	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, 3DR, DDS, NA, 2DA, ACT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.25	0/4324	0.43	0/5854
2	B	0.55	0/249	1.21	4/382 (1.0%)
3	C	0.55	0/297	1.37	4/454 (0.9%)
All	All	0.30	0/4870	0.61	8/6690 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	214	DG	O4'-C4'-C3'	-8.29	101.03	106.00
2	B	108	DG	O4'-C1'-N9	7.35	113.14	108.00
3	C	214	DG	C1'-O4'-C4'	-7.23	102.87	110.10
3	C	206	DG	O4'-C4'-C3'	-5.62	102.25	104.50
2	B	108	DG	C1'-O4'-C4'	-5.38	104.72	110.10
2	B	107	DG	O4'-C1'-N9	-5.34	104.26	108.00
2	B	106	DC	O4'-C1'-N1	-5.17	104.38	108.00
3	C	212	DT	O4'-C1'-N1	-5.07	104.45	108.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4236	0	4277	93	0
2	B	242	0	134	2	0
3	C	278	0	155	4	0
4	A	29	0	12	1	0
5	A	1	0	0	0	0
6	A	12	0	9	0	0
6	C	8	0	6	0	0
7	A	30	0	40	11	0
7	B	12	0	16	6	0
8	A	4	0	0	0	0
9	A	112	0	0	4	0
9	B	23	0	0	2	0
9	C	26	0	0	1	0
All	All	5013	0	4649	104	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (104) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:ARG:HH11	1:A:651:ARG:HH12	1.18	0.90
1:A:650:PRO:HB2	1:A:651:ARG:HE	1.34	0.90
4:A:1:DDS:O2B	9:A:846:HOH:O	2.00	0.79
1:A:317:MET:HB2	7:A:6:GOL:H2	1.67	0.75
1:A:649:VAL:HG11	1:A:652:GLU:HB3	1.72	0.72
7:B:4:GOL:H12	9:B:113:HOH:O	1.90	0.72
1:A:503:ILE:HD11	1:A:522:LEU:HD13	1.72	0.70
1:A:643:ALA:HB2	1:A:662:ALA:HB2	1.74	0.69
1:A:557:THR:OG1	1:A:561:HIS:HE1	1.75	0.68
1:A:636:ARG:HH11	1:A:651:ARG:NH1	1.92	0.66
1:A:563:ARG:HG3	7:A:6:GOL:H31	1.77	0.65
2:B:107:DG:H21	7:B:8:GOL:H32	1.62	0.65
1:A:771:ARG:O	1:A:774:GLU:HG2	1.96	0.65
7:B:4:GOL:H32	9:B:161:HOH:O	1.97	0.64
1:A:549:LEU:HD22	1:A:560:LEU:HD21	1.80	0.64
1:A:650:PRO:O	1:A:651:ARG:HG3	1.98	0.63
1:A:557:THR:HG1	1:A:561:HIS:HE1	1.46	0.61
1:A:302:PRO:HB2	1:A:328:ARG:HD3	1.83	0.60
1:A:641:GLU:O	1:A:645:TRP:CD1	2.55	0.60
1:A:627:ASN:O	1:A:631:VAL:HG23	2.01	0.60
1:A:380:LEU:HD12	1:A:416:LEU:HD12	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:210:DC:H2'	3:C:211:DG:C8	2.37	0.60
1:A:636:ARG:NH1	1:A:651:ARG:HH12	1.96	0.59
1:A:563:ARG:CG	7:A:6:GOL:H31	2.34	0.58
1:A:315:GLU:HB3	7:A:6:GOL:O2	2.04	0.57
1:A:380:LEU:CD1	1:A:416:LEU:HD12	2.33	0.57
1:A:609:LEU:HG	1:A:821:VAL:HG23	1.87	0.56
1:A:650:PRO:HB2	1:A:651:ARG:NE	2.14	0.56
1:A:500:LEU:HD21	1:A:526:HIS:HB2	1.88	0.56
1:A:737:VAL:HG11	7:A:7:GOL:H32	1.88	0.55
1:A:297:ALA:HB2	1:A:331:ARG:HD3	1.89	0.55
7:B:8:GOL:H12	9:C:81:HOH:O	2.07	0.54
1:A:561:HIS:O	7:A:6:GOL:H32	2.08	0.54
1:A:780:LEU:HD11	1:A:790:GLU:HB2	1.92	0.51
1:A:801:ARG:O	1:A:805:GLU:HG2	2.10	0.51
1:A:354:LYS:O	1:A:358:VAL:HG23	2.10	0.51
1:A:470:LEU:O	1:A:474:VAL:HG23	2.10	0.51
1:A:317:MET:CB	7:A:6:GOL:H2	2.39	0.51
1:A:822:GLY:HA3	1:A:830:ALA:O	2.12	0.50
1:A:650:PRO:CB	1:A:651:ARG:HE	2.17	0.50
1:A:785:ASP:OD1	1:A:786:GLU:HG3	2.12	0.50
1:A:297:ALA:CB	1:A:331:ARG:HD3	2.42	0.49
1:A:435:ARG:HB3	1:A:436:PRO:HD3	1.95	0.49
1:A:613:GLN:HG2	1:A:638:ILE:HD11	1.93	0.49
1:A:728:ARG:NH2	1:A:747:MET:HE3	2.29	0.48
3:C:204:3DR:H2''	3:C:205:DT:H73	1.96	0.48
1:A:299:TRP:CG	1:A:300:PRO:HA	2.47	0.48
1:A:585:PRO:HB2	1:A:591:GLY:HA2	1.96	0.48
1:A:526:HIS:O	1:A:529:VAL:HG13	2.14	0.48
1:A:678:LEU:O	1:A:682:LEU:HB2	2.12	0.48
1:A:649:VAL:CG1	1:A:652:GLU:HB3	2.43	0.47
1:A:649:VAL:HG21	1:A:657:LEU:CD1	2.44	0.47
1:A:694:GLU:HA	1:A:694:GLU:OE2	2.15	0.47
1:A:563:ARG:HG2	7:A:6:GOL:H12	1.96	0.47
1:A:445:GLU:O	1:A:561:HIS:HD2	1.97	0.47
1:A:643:ALA:HB2	1:A:662:ALA:CB	2.45	0.46
1:A:585:PRO:O	1:A:595:ARG:HG2	2.16	0.46
1:A:492:ARG:O	1:A:496:ASP:HB2	2.16	0.45
1:A:639:HIS:HB2	1:A:659:ARG:NE	2.30	0.45
1:A:613:GLN:CG	1:A:638:ILE:HD11	2.47	0.45
1:A:631:VAL:HG13	1:A:636:ARG:HB2	1.99	0.45
1:A:721:GLU:HA	1:A:726:ARG:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:ALA:O	1:A:665:ILE:HG13	2.16	0.44
1:A:637:ASP:HB3	1:A:640:THR:OG1	2.17	0.44
9:A:123:HOH:O	7:B:8:GOL:H31	2.17	0.44
1:A:347:GLU:HA	1:A:368:PRO:HD2	1.98	0.44
1:A:392:ARG:HD3	1:A:392:ARG:HA	1.71	0.44
1:A:579:PRO:HB2	7:A:834:GOL:H2	1.99	0.44
1:A:658:MET:CE	1:A:658:MET:HA	2.47	0.44
1:A:669:VAL:HG21	1:A:696:TYR:CE2	2.53	0.44
1:A:483:ASN:H	1:A:489:GLN:HE22	1.66	0.44
1:A:520:GLU:O	1:A:523:ARG:HB2	2.18	0.43
1:A:576:SER:O	3:C:208:DG:H4'	2.17	0.43
1:A:673:MET:HG3	1:A:677:ARG:HB3	1.99	0.43
1:A:636:ARG:NH1	1:A:651:ARG:NH1	2.62	0.43
1:A:743:ALA:HA	1:A:746:ARG:NH2	2.33	0.43
1:A:616:LEU:HD11	1:A:666:ASN:HB3	2.01	0.43
1:A:751:MET:HB3	1:A:752:PRO:HD3	1.99	0.43
1:A:382:PRO:HD2	9:A:151:HOH:O	2.18	0.43
3:C:205:DT:H2''	3:C:206:DG:H5'	2.01	0.43
1:A:665:ILE:O	1:A:669:VAL:HG23	2.19	0.43
1:A:401:GLU:CD	1:A:403:GLY:H	2.22	0.43
1:A:800:ALA:HB2	1:A:823:ILE:HD11	2.01	0.43
1:A:335:ALA:HA	1:A:336:PRO:HD3	1.89	0.42
1:A:650:PRO:HG2	1:A:651:ARG:H	1.84	0.42
1:A:423:GLU:OE1	1:A:727:ARG:NH2	2.51	0.42
1:A:397:GLU:H	1:A:408:LEU:HD13	1.85	0.42
1:A:526:HIS:HA	1:A:527:PRO:HD3	1.88	0.41
1:A:367:LEU:HA	1:A:368:PRO:HD3	1.84	0.41
1:A:712:GLU:HG2	1:A:715:ARG:HH21	1.85	0.41
7:A:836:GOL:H2	9:A:100:HOH:O	2.20	0.41
1:A:611:TYR:HB3	1:A:614:ILE:HB	2.01	0.41
1:A:542:LYS:HA	1:A:546:ILE:HB	2.01	0.41
1:A:628:LEU:HD12	1:A:628:LEU:HA	1.91	0.41
2:B:107:DG:N2	7:B:8:GOL:H32	2.32	0.41
1:A:787:LEU:HD12	1:A:787:LEU:HA	1.89	0.41
1:A:301:PRO:HG3	1:A:326:ALA:HB3	2.02	0.41
1:A:327:ALA:HA	1:A:331:ARG:O	2.20	0.41
1:A:473:GLU:OE1	1:A:473:GLU:HA	2.21	0.41
1:A:669:VAL:HG21	1:A:696:TYR:CZ	2.56	0.40
1:A:666:ASN:O	1:A:670:LEU:HD13	2.21	0.40
1:A:638:ILE:O	1:A:642:THR:N	2.31	0.40
1:A:763:LEU:HD11	1:A:767:LYS:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:PRO:CB	7:A:834:GOL:H2	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	530/540 (98%)	509 (96%)	19 (4%)	2 (0%)	39 43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	647	PHE
1	A	586	VAL

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	432/441 (98%)	417 (96%)	15 (4%)	43 53

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	346	LYS

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Mol	Chain	Res	Type
1	A	392	ARG
1	A	416	LEU
1	A	487	ARG
1	A	522	LEU
1	A	638	ILE
1	A	646	MET
1	A	649	VAL
1	A	651	ARG
1	A	657	LEU
1	A	658	MET
1	A	708	GLU
1	A	713	GLU
1	A	787	LEU
1	A	832	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	384	ASN
1	A	489	GLN
1	A	561	HIS
1	A	565	ASN
1	A	754	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	2DA	B	112	3,2	14,22,23	1.07	1 (7%)	13,31,34	2.62	4 (30%)
3	3DR	C	204	3	7,11,12	0.39	0	8,14,17	1.00	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2DA	B	112	3,2	-	0/3/18/19	0/3/3/3
3	3DR	C	204	3	-	0/3/15/16	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	112	2DA	C5-C4	3.07	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	112	2DA	N3-C2-N1	-7.81	122.92	128.89
2	B	112	2DA	C4-C5-N7	-2.41	107.26	109.48
2	B	112	2DA	C2-N1-C6	2.09	122.51	118.77
2	B	112	2DA	C3'-C2'-C1'	3.16	106.24	102.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	204	3DR	1	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.



## 5.6 Ligand geometry

Of 18 ligands modelled in this entry, 5 are monoatomic - leaving 13 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	DDS	A	1	5	23,31,31	0.97	1 (4%)	28,48,48	2.02	6 (21%)
6	ACT	A	2	-	1,3,3	1.29	0	0,3,3	0.00	-
6	ACT	A	3	-	1,3,3	1.40	0	0,3,3	0.00	-
6	ACT	A	5	-	1,3,3	1.38	0	0,3,3	0.00	-
7	GOL	A	6	-	5,5,5	0.40	0	5,5,5	0.32	0
7	GOL	A	7	-	5,5,5	0.37	0	5,5,5	0.18	0
7	GOL	A	834	-	5,5,5	0.35	0	5,5,5	0.21	0
7	GOL	A	835	-	5,5,5	0.32	0	5,5,5	0.25	0
7	GOL	A	836	-	5,5,5	0.35	0	5,5,5	0.20	0
7	GOL	B	4	-	5,5,5	0.29	0	5,5,5	0.43	0
7	GOL	B	8	-	5,5,5	0.34	0	5,5,5	0.24	0
6	ACT	C	1	-	1,3,3	1.41	0	0,3,3	0.00	-
6	ACT	C	6	-	1,3,3	1.65	0	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DDS	A	1	5	-	0/18/31/31	0/3/3/3
6	ACT	A	2	-	-	0/0/0/0	0/0/0/0
6	ACT	A	3	-	-	0/0/0/0	0/0/0/0
6	ACT	A	5	-	-	0/0/0/0	0/0/0/0
7	GOL	A	6	-	-	0/4/4/4	0/0/0/0
7	GOL	A	7	-	-	0/4/4/4	0/0/0/0
7	GOL	A	834	-	-	0/4/4/4	0/0/0/0
7	GOL	A	835	-	-	0/4/4/4	0/0/0/0
7	GOL	A	836	-	-	0/4/4/4	0/0/0/0
7	GOL	B	4	-	-	0/4/4/4	0/0/0/0
7	GOL	B	8	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ACT	C	1	-	-	0/0/0/0	0/0/0/0
6	ACT	C	6	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1	DDS	C5-C4	3.20	1.47	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	DDS	N3-C2-N1	-6.75	123.72	128.89
4	A	1	DDS	PB-O3B-PG	-3.87	119.68	132.67
4	A	1	DDS	PB-O3A-PA	-3.44	123.06	132.73
4	A	1	DDS	C4-C5-N7	-2.97	106.75	109.48
4	A	1	DDS	O3G-PG-O2G	2.00	115.00	107.38
4	A	1	DDS	C3'-C2'-C1'	3.04	106.10	102.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	DDS	1	0
7	A	6	GOL	7	0
7	A	7	GOL	1	0
7	A	834	GOL	2	0
7	A	836	GOL	1	0
7	B	4	GOL	2	0
7	B	8	GOL	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	534/540 (98%)	-0.01	28 (5%) 31 34	20, 47, 111, 167	0
2	B	11/12 (91%)	-0.74	0 100 100	21, 27, 70, 73	0
3	C	13/16 (81%)	-0.72	0 100 100	22, 28, 49, 120	1 (7%)
All	All	558/568 (98%)	-0.04	28 (5%) 32 36	20, 46, 111, 167	1 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	648	GLY	15.6
1	A	647	PHE	7.5
1	A	650	PRO	5.8
1	A	689	ALA	5.5
1	A	644	SER	4.2
1	A	499	GLY	3.8
1	A	683	ALA	3.5
1	A	695	ARG	3.2
1	A	645	TRP	3.2
1	A	692	PHE	3.1
1	A	696	TYR	3.0
1	A	660	ARG	2.8
1	A	688	GLU	2.8
1	A	638	ILE	2.7
1	A	657	LEU	2.7
1	A	643	ALA	2.7
1	A	691	ALA	2.7
1	A	326	ALA	2.6
1	A	704	ARG	2.6
1	A	646	MET	2.5
1	A	325	ALA	2.4
1	A	631	VAL	2.4
1	A	694	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	329	GLY	2.3
1	A	681	GLU	2.1
1	A	333	HIS	2.1
1	A	503	ILE	2.0
1	A	297	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	2DA	B	112	20/21	0.98	0.11	-	24,30,35,35	0
3	3DR	C	204	11/12	0.97	0.14	-	44,53,81,84	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	ACT	A	5	4/4	0.57	0.27	25.46	69,69,70,71	0
7	GOL	A	836	6/6	0.82	0.39	25.02	47,60,63,65	0
7	GOL	A	6	6/6	0.91	0.34	24.79	34,37,38,43	0
8	NA	A	4	1/1	0.82	0.33	22.57	69,69,69,69	0
7	GOL	B	8	6/6	0.84	0.22	13.72	56,65,66,67	0
6	ACT	C	6	4/4	0.76	0.19	8.75	44,46,47,48	0
7	GOL	A	835	6/6	0.78	0.20	2.78	63,68,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	NA	A	837	1/1	0.95	0.12	2.25	39,39,39,39	0
7	GOL	A	834	6/6	0.98	0.10	0.30	31,31,33,34	0
4	DDS	A	1	29/29	0.89	0.12	-0.68	49,72,94,271	0
6	ACT	A	3	4/4	0.81	0.14	-	40,49,51,52	0
6	ACT	A	2	4/4	0.91	0.18	-	59,60,60,60	4
8	NA	A	838	1/1	0.70	0.17	-	86,86,86,86	0
6	ACT	C	1	4/4	0.86	0.19	-	55,58,59,60	0
7	GOL	A	7	6/6	0.72	0.28	-	35,38,39,40	6
8	NA	A	839	1/1	0.83	0.30	-	71,71,71,71	0
7	GOL	B	4	6/6	0.82	0.20	-	37,46,52,56	0
5	MG	A	833	1/1	0.91	0.05	-	73,73,73,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.